

Connection Between Continuous and Discrete Time Quantum Walks on d -Dimensional Lattices; Extensions to General Graphs

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Abstract

I obtain the dynamics of the continuous time quantum walk on a d -dimensional lattice, with periodic boundary conditions, as an appropriate limit of the dynamics of the discrete time quantum walk on the same lattice. This extends the main result of [8] which proved this limit for the case of the quantum walk on the infinite line and the quantum cellular automaton proposed in [1]. By highlighting the main features of the limiting procedure, I then extend it to general graphs. For a given discrete time quantum walk on a general graph, I single out the type of continuous dynamics (Hamiltonians) that can be obtained as a limit of the discrete time dynamics.

1 Generalities on quantum walks; continuous and discrete time

Consider a graph $G := \{V, E\}$ with a set of vertices V of cardinality N and a set of edges E . We assume G to be undirected and without self-loops. In the interval of time Δt a certain fraction $\gamma\Delta t$ of a quantity p_j leaves the location of the j -th vertex to move to a neighboring vertex k . The quantity p_j , $j = 1, \dots, N$, at time $t + \Delta t$ is given by¹

$$p_j(t + \Delta t) = p_j(t) - \deg(j)\gamma\Delta t p_j(t) + \sum_{(k,j) \in E} \gamma\Delta t p_k(t). \quad (1)$$

Define \vec{p} the N -vector whose components are the p_j 's quantities, and L the *Laplacian* matrix defined by $L_{jj} = -\deg(j)$, $L_{jk} = 1$ if $(j, k) \in E$ and $L_{jk} = 0$ otherwise. L is

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¹The rate γ may depend on time and we could have allowed it to depend on the location j . In the latter case though we cannot choose a Laplacian matrix L (see later) to be symmetric.

symmetric and, except for the elements on the diagonal, coincides with the adjacency matrix A , that is, $A_{jk} := L_{jk}$, when $j \neq k$ and $A_{jk} = 0$ if $j = k$. Taking the limit $\Delta t \rightarrow 0$ in (1) one obtains the differential equation for the *classical continuous-time random walk* (CTRW).

$$\frac{d}{dt}\vec{p} = \gamma L\vec{p}. \quad (2)$$

The reason to call this model a random walk is that the $p_j(t)$'s may represent the probability of a walker to be in position j at time t . A continuous-time *quantum random walk* (CTQW) (see [4]) is obtained by quantizing equation (2). One replaces \vec{p} with a complex N -vector representing the state of a quantum system, while L is taken as the Hamiltonian determining the evolution according to the Schrödinger equation

$$i\dot{\psi} = \gamma L\psi, \quad (3)$$

with $|\psi_j|^2$ representing the probability of the quantum system being in the basis state $|j\rangle$. This definition can be generalized by using an Hamiltonian different from L which respects the topology of the graph G , that is elements different from zero correspond to edges in the graph. For example one can use the adjacency matrix A instead of L in (3).²

The *classical discrete-time random walk* (DTRW) is obtained by discretizing equation (2) and therefore it is given by equation (1). The CTRW is obtained from the DTRW by taking the limit $\Delta t \rightarrow 0$ in equation (1) as seen above. To define the *discrete time quantum walk* (DTQW), we would like to write an equation of the form

$$\psi(t+1) = U\psi(t), \quad (4)$$

with ψ the state of a quantum system and U a unitary operator representing a (closed) quantum evolution. We also would like to have a U which respects the structure of the underlying graph G , i.e., U_{jk} , with $j \neq k$ is different from zero if and only if there exists an edge (j, k) in E . Unfortunately, only special graphs have the property that such a unitary matrix exists [7]. In order to give a definition which is suitable for any graph one proceeds as follows.

Let \mathcal{V} be the Hilbert space spanned by the orthonormal states $\{|j\rangle\}$, with $j \in V$. Let \mathcal{E} be the subspace of $\mathcal{V} \otimes \mathcal{V}$ spanned by $|j, k\rangle$ with $(j, k) \in E$. The basis state $|j, k\rangle$ represents the state of a walker which is currently in vertex j and is moving to vertex k , i.e., j and k are the *present* and *future* location of the walker, respectively. On the space \mathcal{E} , the evolution U of the DTQW is of the form $U = W\tilde{C}$. The operation \tilde{C} , called *coin tossing*, is of the form

$$\tilde{C} = \sum_{j \in V} |j\rangle\langle j| \otimes Q_j, \quad (5)$$

where Q_j is a unitary transformation on \mathcal{V} , depending on j . The subspace spanned by the states corresponding to the neighboring vertices of j (and therefore its orthogonal

²In this case, if G is a regular graph, i.e., $\deg(j)$ is the same for every j in V , the corresponding dynamics would differ from the ones of (3) only by a physically unimportant phase factor.

complement) is invariant under Q_j . The operation W is any unitary which transforms the elements $|j, k\rangle$ as $W|j, k\rangle = |k, r\rangle$, for some $|k, r\rangle \in \mathcal{E}$, i.e., it moves the future state in the present state position. One possibility is the *swap* operation, defined by $W|j, k\rangle = |k, j\rangle$, since $|j, k\rangle \in \mathcal{E} \leftrightarrow |k, j\rangle \in \mathcal{E}$.

If the graph G is regular, one can give a definition which makes the coin's role more transparent. We call this quantum walk the *coined* DTQW. It is defined as follows. Let m be the degree of G and consider a (coin) space \mathcal{C} spanned by orthogonal states $\{|c_1\rangle, \dots, |c_m\rangle\}$ each representing the result of a coin tossing. Denote by $n_j(c_k)$, $j = 1, \dots, N$, $k = 1, \dots, m$, an element in V if a coin result c_k induces a transition from j to it. The coined DTQW evolves on $\mathcal{C} \otimes \mathcal{V}$ as $R = SC \otimes \mathbf{1}$, where C is a unitary (coin tossing) operation on \mathcal{C} , $\mathbf{1}$ is the identity on the walker space \mathcal{V} and S is a *controlled shift* defined by

$$S|c_k, j\rangle = |c_k, n_j(c_k)\rangle. \quad (6)$$

The coined DTQW, defined in the case of a regular graph, is a special case of the more general DTQW defined above, when the coin operations Q_j in (5) are essentially independent of j and W takes a special form. To be more specific, let C in the coined DTQW be defined by

$$C|c_k\rangle := \sum_{l=1}^m \alpha_{lk}|c_l\rangle. \quad (7)$$

Then choose Q_j in (5) as

$$Q_j|n_j(c_k)\rangle = \sum_{l=1}^m \alpha_{lk}|n_j(c_l)\rangle \quad (8)$$

(notice the coefficients α_{lk} are independent of j). The transformation W of the DTQW is chosen as

$$W|j, n_j(c_k)\rangle = |n_j(c_k), n_{n_j(c_k)}(c_k)\rangle. \quad (9)$$

With these choices, the dynamics of the DTQW on \mathcal{E} are equivalent to the dynamics of the coined DTQW on $\mathcal{C} \otimes \mathcal{V}$. In fact, using the isomorphism $\chi : \mathcal{C} \otimes \mathcal{V} \rightarrow \mathcal{E}$ defined by

$$\chi|c_k, j\rangle = |j, n_j(c_k)\rangle, \quad (10)$$

we have that $\chi S(C \otimes \mathbf{1}) = W\tilde{C}\chi$. In fact, a straightforward computation shows

$$\chi S(C \otimes \mathbf{1})|c_k, j\rangle = \sum_{l=1}^m \alpha_{lk}|n_j(c_l), n_{n_j(c_l)}(c_l)\rangle = W\tilde{C}\chi|c_k, j\rangle. \quad (11)$$

Having defined the DTQW and the CTQW the question remains on whether the CTQW can be obtained as a limit of the DTQW on the same graph. This is a fundamental question which was posed in [6] and has received much attention recently (see, e.g., [2], [8] and references therein). It is motivated, among other things, by the fact that CTQW and DTQW on the same graphs have showed similar behavior in several applications. Since the DTQW evolves on an higher dimensional space as compared with the CTQW, the

procedure to obtain the CTQW from the DTQW should involve not only an appropriate limit but also some sort of a projection of the dynamics onto a lower dimensional space. This work was done in [8] for the quantum walk on the infinite line. In this paper, I extend and somewhat simplify the calculation in [8] to prove the same limit for the coined DTQW on a d -dimensional lattice with periodic boundary conditions. In particular for $d = 1$, I obtain the CTQW from the DTQW for the cycle. I then observe that this generalization is only an example of a general procedure that I then extend to general graphs. I formalize this procedure by describing the set of Hamiltonian dynamics for the CTQW which can be obtained by a limit of the dynamics of the DTQW (cf. Theorem 1). In the following, I shall consider only coined DTQW.

The paper is organized as follows. In Section 2 I describe in detail the quantum walk on a d -lattice. The d -lattice is the Cartesian product of d cycle graphs. If the transition from discrete to continuous is obtained for each factor of a product graph then it carries over to the whole graph (cf. end of Section 2 and Remark 2.1). Therefore, it is enough to restrict ourselves to the cycle. I prove the transition from DTQW to CTQW for the cycle in Section 3. The calculation in this section can be carried over to other quantum walks. Moreover, even for the case of the cycle alternative limiting procedures to obtain the CTQW from the DTQW can be devised as discussed in Remark 4.1. In Section 4, I extend the procedure to general coined quantum walks. I characterize in Theorem 1 the set of Hamiltonians on the space $\mathcal{E} \otimes \mathcal{V}$ whose dynamics can be obtained as a limit of the one of the DTQW. I give an example in section 5 and conclude in section 6.

2 Quantum walks on d -dimensional lattices

Consider a coined DTQW on a d -dimensional lattice whose set of vertices V is given by $V = \{0, 1, \dots, N - 1\}^d$. If $\tilde{\mathcal{V}} := \text{span } \{|0\rangle, |1\rangle, \dots, |N - 1\rangle\}$, is the Hilbert space associated with $\{0, 1, \dots, N - 1\}$, the walker Hilbert space for this graph is $\mathcal{V} = \otimes^d \tilde{\mathcal{V}}$, which is spanned by the orthonormal vectors $|j_1, \dots, j_d\rangle$, $j_1, \dots, j_d = 0, 1, \dots, N - 1$, which represent vertices of the graph with coordinates j_1, \dots, j_d . In the graph G , the vertex labeled by (j_1, \dots, j_d) has $2d$ neighbors each differing by (j_1, \dots, j_d) by only one coordinate and with (Hamming) distance 1, i.e., of the form $(j_1, \dots, j_k \pm 1, \dots, j_d)$, where the ± 1 operation has to be intended mod N . Let \tilde{G} be the graph representing the cycle with N nodes. G is the product of d copies of \tilde{G} . Its adjacency matrix is

$$A := \sum_{l=1}^d \tilde{A}^{(l)}, \quad (12)$$

where $\tilde{A}^{(l)}$ is the tensor product of d , $N \times N$ identity matrices except in the l -th position which is occupied by the adjacency matrix of the cycle \tilde{A} .³ \tilde{A} is given by $\tilde{A} = F + F^T$,

³There are several definitions of product of d graphs. Here we intend the *Cartesian product* of d graphs $G_l \equiv (V_l, E_l)$, $l = 1, \dots, d$ which is defined as the graph $G \equiv (V, E)$ having the set of vertexes V equal to the Cartesian product $V := V_1 \times V_2 \times \dots \times V_d$ and set of edges E such that

where the circulant matrix F is defined as

$$F := \begin{pmatrix} 0 & 0 & \cdot & \cdot & \cdot & 0 & 1 \\ 1 & 0 & \cdot & \cdot & \cdot & 0 & 0 \\ 0 & 1 & \cdot & \cdot & \cdot & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & \cdot & \cdot & \cdot & \cdot & 1 & 0 \end{pmatrix}. \quad (13)$$

The Laplacian is given by

$$L := -\deg(G)\mathbf{1} + A = -2d\mathbf{1} + A, \quad (14)$$

and the solution of the corresponding Schrodinger equation is $\psi(t) = X(t)\psi(0)$, with $X(t) = X_1(t) \otimes \cdots \otimes X_d(t)$, where X_l is the solution of the Schrödinger operator equation corresponding to the l -th graph (cycle)

$$i\dot{X}_l = \gamma \tilde{L} X_l, \quad X_l(0) = \mathbf{1}, \quad (15)$$

where $\tilde{L} = -2\mathbf{1} + \tilde{A}$ is the Laplacian corresponding to a single cycle.

To construct a coined DTQW on the d -dimensional lattice, we have to introduce a coin space \mathcal{C} which is spanned by $2d$ basis vectors, each corresponding to a different coin result. We choose the basis so that the vectors corresponding to the same degree of freedom are placed one after the other. For example, for a 2-dimensional lattice, \mathcal{C} is spanned by the ordered basis $\{| \rightarrow \rangle, | \leftarrow \rangle, | \uparrow \rangle, | \downarrow \rangle\}$, which induce a right, left, up and down motion, respectively. The dynamics of the coined DTQW on $\mathcal{C} \otimes \mathcal{V}$ is given by $SC \otimes \mathbf{1}_{N^d \times N^d}$ where C is a coin transformation on \mathcal{C} and S is the controlled shift. S is a $2dN^d \times 2dN^d$ block diagonal matrix with d , $2N^d \times 2N^d$ -dimensional, blocks each corresponding to one degree of freedom in the coin space. The l -th block is given by

$$S^{(l)} = \begin{pmatrix} F^{(l)} & 0 \\ 0 & F^{(l)T} \end{pmatrix}, \quad (16)$$

where $F^{(l)}$ ($F^{(l)T}$) is the tensor product of d , $N \times N$ identity matrices, except in the l -th position which is occupied by F (F^T) in (13). It represents a forward (backward) motion

$((u_1, u_2, \dots, u_d), (v_1, v_2, \dots, v_d)) \in E$ if and only if all u_j 's are equal to the corresponding v_j 's except for exactly one pair $u_{\bar{j}} \neq v_{\bar{j}}$ which is such that $(u_{\bar{j}}, v_{\bar{j}}) \in E_{\bar{j}}$. The adjacency matrix of such a graph is $A = \sum_{l=1}^d \tilde{A}^{(l)}$ where $\tilde{A}^{(l)}$ is the tensor product of d matrices all equal to the identity, with the one in a generic position r of dimension $|V_r|$, except for the matrix in position l which is equal to the adjacency matrix of the l -th graph. A quick way to see that this is the case is to recall that a definition of adjacency matrix A given by $e_j^T A e_k = 1$ if and only if (j, k) is an edge and $= 0$ otherwise. Here e_j and e_k are the standard basis vectors corresponding the vertexes j and k . A quick calculation of $\langle j_1, \dots, j_d | A | k_1, \dots, k_d \rangle$ shows that this is the case for the above defined matrix. If the graphs G_1, \dots, G_d are all regular, so is the product graph and its degree is the sum of the degrees of the graphs G_1, \dots, G_d .

in the degree of freedom identified by l (for example $l = 1$ (right or left motion), $l = 2$ (upward and downward motion).

The matrix C is, in principle, a general matrix in $U(2d)$ (i.e., $2d \times 2d$ unitary), which depends therefore on $(2d)^2$ real parameters. It is the only element in the dynamics which couples the various degree of freedom of the motion of the DTQW. We would like to obtain the dynamics of the CTQW as an appropriate limit involving the parameters in this matrix and going from discrete to continuous time. Since the dynamics of the CTQW given by (15) is completely decoupled, it is reasonable to restrict our attention to coin transformations which do not couple the various degrees of freedom of the coin. The corresponding matrix C has a block diagonal structure with $d, 2 \times 2$ blocks belonging to $U(2)$. With this restriction, the dynamics of the DTQW also are completely decoupled and we can restrict our attention to only one factor in the product graph, i.e., a cycle. Therefore, in the following, we shall restrict ourselves to a DTQW on a cycle with N vertexes, whose dynamics is given by $S(C \otimes \mathbf{1}_{N \times N})$ with C in $SU(2)$ and

$$S = \begin{pmatrix} F & 0 \\ 0 & F^T \end{pmatrix}. \quad (17)$$

Remark 2.1 In what we have said above, there is no reason to consider the product of cycles with equal number of nodes N , other than notational convenience. More generally, for product graphs, the adjacency matrix always has the form of a sum of adjacency matrices as in (12) and the dynamics of the continuous quantum walks are always decoupled. Therefore if we have a limiting procedure to obtain the dynamics of the CTQW from the DTQW for each factor graph, we can carry this over to the product graph by restricting the dynamics of the coin space in a way that the dynamics on the different factor graphs are decoupled. The same holds for the quantum walk where the Hamiltonian is given by the Laplacian since this only differs from the one corresponding to the adjacency matrix by a physically unimportant multiple of the identity. The important fact is that the Hamiltonian for the product graph has the form (12) (i.e., sum of matrices which are products of the identity on the various spaces except for a local Hamiltonian). There are however Hamiltonians that respect the structure of the product graph but cannot be written this way. For these Hamiltonians the graph has to be considered as a whole.

3 Continuous time quantum walk as limit of discrete time quantum walks on the cycle

Consider the coined DTQW on the cycle and write the coin operation $C \in SU(2)$ as

$$C = Re^{iDx}, \quad (18)$$

with $R := \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}$ and $D := \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$. With x small, $U^2(x) = SC \otimes \mathbf{1}SC \otimes \mathbf{1}$, represents a small perturbation to a transformation $U^2(0) = -\mathbf{1}_2 \otimes \mathbf{1}_N$ (cf. (17) using

the fact that $FF^T = \mathbf{1}_N$) which does not modify the state of the system (except for an unimportant phase factor). Write $e^{iDx} = \mathbf{1}_2 + iDx + O(x^2)$. We write $U^2(x)$ as⁴

$$\begin{aligned} U^2(x) &= S \left(R(\mathbf{1}_2 + iDx + O(x^2)) \otimes \mathbf{1}_N \right) S \left(R(\mathbf{1}_2 + iDx + O(x^2)) \otimes \mathbf{1}_N \right) \quad (19) \\ &= (S(R \otimes \mathbf{1}))^2 + i \left((S(R \otimes \mathbf{1}))^2 D \otimes \mathbf{1} + S(R \otimes \mathbf{1})D \otimes \mathbf{1}S(R \otimes \mathbf{1}) \right) x + O(x^2). \end{aligned}$$

We have already said that $(S(R \otimes \mathbf{1}))^2 = -\mathbf{1}_2 \otimes \mathbf{1}_N$. On the other hand, a direct calculation shows that

$$(S(R \otimes \mathbf{1}))^2 D \otimes \mathbf{1} + S(R \otimes \mathbf{1})D \otimes \mathbf{1}S(R \otimes \mathbf{1}) = \begin{pmatrix} 0 & \mathbf{1} + F^2 \\ \mathbf{1} + F^{2T} & 0 \end{pmatrix}. \quad (20)$$

Therefore, we have

$$U^2(x) = - \left(\mathbf{1} - i \begin{pmatrix} 0 & \mathbf{1} + F^2 \\ \mathbf{1} + F^{2T} & 0 \end{pmatrix} x + O(x^2) \right). \quad (21)$$

If H is the Hamiltonian

$$H := \begin{pmatrix} 0 & \mathbf{1} + F^2 \\ \mathbf{1} + F^{2T} & 0 \end{pmatrix}, \quad (22)$$

then

$$U^2(x) = -e^{-iHx} + O(x^2), \quad (23)$$

i.e., for small perturbations x two iterations of the DTQW give an evolution which (except for the unimportant phase factor -1) corresponds to the continuous evolution by a Hamiltonian H in (22) in the same time x . One obtains an evolution $e^{-i\gamma H t}$ over an arbitrary time t by applying $U^2(x)$ an infinite number of times and, at the same time, letting $x \rightarrow 0$. More specifically, setting $\frac{\tau}{2} = \frac{\gamma t}{x}$ and neglecting the, physically irrelevant factor -1 in (23), we have⁵

$$\lim_{x \rightarrow 0} U^\tau(x) = \lim_{x \rightarrow 0} \left(e^{-iHx} + O(x^2) \right)^{\frac{\gamma t}{x}} = e^{-i\gamma H t}. \quad (25)$$

Therefore, over the interval $[0, t]$ the system evolves according to the Schrödinger equation $i\dot{\psi} = \gamma H\psi$ where H is defined in (22). Defining $\psi := [\psi_R^T, \psi_L^T]^T$, with ψ_R and ψ_L both N -dimensional, we have

$$\dot{\psi}_R = -i\gamma(\mathbf{1} + F^2)\psi_L, \quad (26)$$

⁴Sometimes, when it is clear from the context, we omit the dimension of the identity matrix $\mathbf{1}$.

⁵This limit can be obtained from general properties of the logarithms of matrices (cf. [5] section 6.5). Set $\frac{\gamma t}{x} := m = \frac{\tau}{2}$. The limit in (25) becomes

$$\begin{aligned} \lim_{m \rightarrow \infty} \left(e^{-iH\frac{\gamma t}{m}} + O\left(\frac{1}{m^2}\right) \right)^m &= \lim_{m \rightarrow \infty} \left(\mathbf{1} - iH\frac{\gamma t}{m} + O\left(\frac{1}{m^2}\right) \right)^m = \lim_{m \rightarrow \infty} e^{\log(\mathbf{1} - iH\frac{\gamma t}{m} + O(\frac{1}{m^2}))^m} = \\ &\lim_{m \rightarrow \infty} e^{-m\left(\frac{1}{m}(iH\gamma t - O(\frac{1}{m})) + \frac{1}{2m^2}(iH\gamma t - O(\frac{1}{m}))^2 + \dots\right)} = e^{-i\gamma H t}. \end{aligned} \quad (24)$$

Here we have used the series expansion of the principal logarithm of a matrix $\log(\mathbf{1} - A) = -\sum_{k=1}^{\infty} \frac{1}{k} A^k$.

$$\dot{\psi}_L = -i\gamma(\mathbf{1} + F^{2T})\psi_R. \quad (27)$$

There are special (linear) combinations of ψ_R and ψ_L which evolve according to $i\dot{\Psi} = \pm\gamma A\Psi$ where $A = F + F^T$ is the adjacency matrix of the cycle graph. In particular, define

$$\Psi_{1+} := \psi_R + F\psi_L. \quad (28)$$

Using (26) and (27)

$$\begin{aligned} \dot{\Psi}_{1+} &= -i\gamma \left((F^T F + F^2)\psi_L + F(\mathbf{1} + F^{2T})\psi_R \right) = \\ &-i\gamma \left(F^T(\psi_R + F\psi_L) + F(\psi_R + F\psi_L) \right) = -i\gamma A\Psi_{1+}. \end{aligned} \quad (29)$$

With analogous calculations, after defining

$$\Psi_{2+} := \psi_L + F^T\psi_R, \quad (30)$$

$$\Psi_{1-} := \psi_R - F\psi_L, \quad (31)$$

$$\Psi_{2-} := \psi_L - F^T\psi_R, \quad (32)$$

one finds

$$i\dot{\Psi}_{1,2\pm} = \pm\gamma A\Psi_{1,2\pm}. \quad (33)$$

From these equations, it follows that, defining

$$\Phi_{1,2\pm} := \frac{e^{\pm 2i\gamma t}}{2}\Psi_{1,2\pm}, \quad (34)$$

we have

$$i\dot{\Phi}_{1,2\pm} = \pm\gamma L\Phi_{1,2\pm}, \quad (35)$$

where L is the Laplacian $L = -2\mathbf{1} + A$. These are the dynamics (forward or backward in time) of the corresponding CTQW.

The dynamics of $[\psi_R, \psi_L]^T$ are obtained as the average of dynamics of the CTQW corresponding to the adjacency matrix, i.e., (from (28), (30), (31), (32))

$$\begin{pmatrix} \psi_R \\ \psi_L \end{pmatrix} = \frac{1}{2} \left(\begin{pmatrix} \Psi_{1+} \\ \Psi_{2+} \end{pmatrix} + \begin{pmatrix} \Psi_{1-} \\ \Psi_{2-} \end{pmatrix} \right). \quad (36)$$

4 Extension to general graphs

The calculation presented in the previous section follows the main steps of [8] which we have adapted to the case of the cycle. We have however modified this calculation in several respects. In particular, we have omitted the Fourier transformation (and anti-transformation) step and replaced the calculation (8) of [8] which is based on the algebra of Pauli matrices with a Taylor expansion in a perturbation parameter x . In this form, the treatment highlights the main ideas of the process to obtain the dynamics the CTQW as

an appropriate limit of the coined DTQW and therefore can be generalized. In fact, we will show in this section how this limit can be extended to quantum walks on general graphs and-or CTQW with Hamiltonian different from the Laplacian or the adjacency matrix. The main idea of the calculation in the previous section is to take a *reference trajectory* of the coined DTQW which takes the walk back to its original position (up to an overall phase factor).⁶ Then one perturbs such a trajectory by slightly modifying the coin operation at each step. Let x be a parameter which measures the magnitude of this perturbation. The resulting trajectory will agree with e^{-iHx} for a certain *simulable Hamiltonian* H up to higher order terms $O(x^{1+\delta})$, ($\delta > 0$). Then one repeats this trajectory a number of times which increases as $x \rightarrow 0$ while letting the perturbation go to zero as in (24). The result is an evolution of the type $e^{-i\gamma Ht}$ for some scalar γ . The Hamiltonian H acts on a $c \times N$ space where c is the dimension of the coin space and N is the dimension of the walker space (i.e., the number of vertices of the graph) while we would like to obtain an evolution according to an Hamiltonian \tilde{H} acting on N -dimensional space. However, if the simulable Hamiltonian H has N eigenvalues coinciding with the ones of \tilde{H} , by a change of coordinates we can isolate a subspace of $\mathcal{C} \otimes \mathcal{H}$ where the evolution coincides with the one determined by \tilde{H} . This is meaning of the calculations in (28)-(36).⁷

Remark 4.1 We remark that the above procedure can be used not only to obtain the CTQW as a limit of the coined DTQW for new graphs (as we shall see in the following) but also to obtain alternative procedures for the case of the cycle. For example, consider the reference trajectory $S^N = \mathbf{1}$ with S given in (17) and perturb it as

$$S^N \rightarrow Se^{Ex} \otimes \mathbf{1} S^{N-1} e^{Ex} \otimes \mathbf{1}, \quad (37)$$

with $E := \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}$. A straightforward calculation shows that we have

$$Se^{Ex} \otimes \mathbf{1} S^{N-1} e^{Ex} \otimes \mathbf{1} = \mathbf{1} - iHx + O(x^2) = e^{-iHx} + O(x^2), \quad (38)$$

where H is the same as in (22). Therefore the treatment then goes as after formula (23).

The question at this point is the characterization of the set of simulable Hamiltonians for general coined DTQW. To this purpose we give a more precise definition of simulable Hamiltonian and then describe this set in Theorem 1 below.

Definition 4.2 An Hamiltonian H on the Hilbert space $\mathcal{C} \otimes \mathcal{V}$ (with $c = \dim \mathcal{C}$ and $N = \dim \mathcal{V}$) is called simulable if there exists a parameter x and a sequence of transformations $SC_j e^{E_j x} \otimes \mathbf{1}$, with $C_j \in U(c)$, $E_j \in u(c)$, $j = 1, \dots, m$, such that

$$\prod_{j=1}^m SC_j e^{E_j f_j(x)} \otimes \mathbf{1} = e^{-iHx} + O(x^{1+\delta}), \quad (39)$$

⁶Note that such a trajectory always exists. As the matrix S in (6) is a permutation matrix $S^r = \mathbf{1}$ with r the order of S . That is: by taking r steps with the coin operation C equal to the identity we come back to the original position of the walk.

⁷In this case, in fact, there are 4 possible subspaces and, at the limit, the dynamics of the DTQW gives 4 copies of the dynamics of CTQW, 2 forward in time and 2 backward in time.

for some $\delta > 0$, strictly increasing smooth functions, f_j , $f_j(0) = 0$ and $x \in [0, \epsilon]$, for some $\epsilon > 0$.

If H is simulable, then one can use a sequence of steps of the DTQW and perform a limit procedure as in (24) to obtain the dynamics corresponding to H . In particular, using (39), one obtains

$$\lim_{x \rightarrow 0} \left(\prod_{j=1}^m SC_j e^{E_j f_j(x)} \otimes \mathbf{1} \right)^{\frac{\gamma t}{x}} = \lim_{x \rightarrow 0} \left(e^{-iHx} + O(x^{1+\delta}) \right)^{\frac{\gamma t}{x}} = e^{-iH\gamma t} \quad (40)$$

Theorem 1 Let r be the order of the matrix S of a coined DTQW, and consider the set

$$\mathcal{F} = \{u(c) \otimes \mathbf{1}_N, Su(c) \otimes \mathbf{1}_N S^{r-1}, S^2 u(c) \otimes \mathbf{1}_N S^{r-2}, \dots, S^{r-1} u(c) \otimes \mathbf{1}_N S\}. \quad (41)$$

Then, the set of simulable Hamiltonian is (modulo i) the Lie algebra generated by \mathcal{F} .

We denote by ‘Sim’ the set of simulable Hamiltonians and by \mathcal{L} the Lie algebra generated by \mathcal{F} .⁸ The statement of the Theorem says that

$$i \text{ Sim } = \mathcal{L} \quad (42)$$

Proof. First, we show that $i \text{ Sim } \subseteq \mathcal{L}$. Assume $H \in \text{Sim}$ so that (39) holds. For every x in $[0, \epsilon)$ the left hand side belongs to the Lie group corresponding to the Lie algebra \mathcal{L} , which we denote by $e^{\mathcal{L}}$. To see this, we first observe that $e^{\mathcal{L}}$ has the property

Property (a):

$$X \in e^{\mathcal{L}} \Leftrightarrow S^k X S^{-k} \in e^{\mathcal{L}},$$

for every integer k .

This property holds for the Lie algebra \mathcal{L} (i.e., with $e^{\mathcal{L}}$ replaced by \mathcal{L}) and carries over to the Lie group $e^{\mathcal{L}}$.⁹

Notice that the left hand side of (39) (as well as the right hand side) is equal to the identity when $x = 0$. If $m = 1$ in (39) then the left hand side is a curve in $e^{\mathcal{L}}$ for every $x \in [0, \epsilon)$, $T = T(x)$, with $T(0) = \mathbf{1}$. This is true even if $m \geq 2$. To see this, we proceed by induction on m , using *Property (a)*. From $\prod_{j=1}^m SC_j \otimes \mathbf{1}_N = \mathbf{1}_{cN}$, we obtain $SC_1 \otimes \mathbf{1} = \prod_{j=m}^2 (C_j^\dagger \otimes \mathbf{1} S^\dagger)$, and therefore we have

$$\prod_{j=1}^m SC_j e^{E_j f_j(x)} \otimes \mathbf{1} = \prod_{j=m}^2 (C_j^\dagger \otimes \mathbf{1} S^\dagger) e^{E_1 f_1(x)} \otimes \mathbf{1} \prod_{j=2}^m SC_j e^{E_j f_j(x)} \otimes \mathbf{1} := L_m(x). \quad (43)$$

⁸Note this coincides with the dynamical Lie algebra studied in [3] which determines the set of reachable states for a DTQW on the cycle seen as a control system.

⁹To prove that the property holds for \mathcal{L} just observe that it holds for the set \mathcal{F} in (41) and it is preserved under linear combination and Lie bracket of two elements of the Lie algebra.

Define $L_1(x) = e^{E_1 f_1(x)} \otimes \mathbf{1}$ which is in $e^{\mathcal{L}}$. We have

$$L_{m+1}(x) = C_{m+1}^\dagger \otimes \mathbf{1} S^\dagger L_m(x) S C_{m+1} \otimes \mathbf{1} e^{E_{m+1} f_{m+1}(x)} \otimes \mathbf{1}. \quad (44)$$

$S^\dagger L_m(x) S \in e^{\mathcal{L}}$ because of *Property (a)* and taking the product with element in $e^{\mathcal{L}}$ we obtain an element in $e^{\mathcal{L}}$ because of the group property. In conclusion the left hand side of (39) is a smooth curve $T(x)$ in $e^{\mathcal{L}}$, with $T(0) = \mathbf{1}$. From

$$T(x) = e^{-iHx} + O(x^{1+\delta}), \quad (45)$$

taking the derivative with respect to x at $x = 0$ we obtain $-iH = \dot{T}(0)$, i.e., $-iH$ is an element of the Lie algebra \mathcal{L} . This conclude the proof that $i \text{ Sim } \subseteq \mathcal{L}$.

To prove that $\mathcal{L} \subseteq i \text{ Sim }$ we prove two facts

1.

$$\mathcal{F} \subseteq i \text{ Sim }$$

2. $i \text{ Sim }$ is a (real) Lie algebra.¹⁰

From these two facts, since, by definition, \mathcal{L} is the smallest subalgebra of $u(cN)$ containing \mathcal{F} , it follows that $\mathcal{L} \subseteq i \text{ Sim }$. The proof of 1. is almost obvious. If $-iH \in \mathcal{F}$ then $e^{-iHx} = S^k e^{Lx} \otimes \mathbf{1} S^{r-k}$ for some $k = 1, \dots, r$, and this can be written in the form (39) by choosing $m = r$, $C_j = \mathbf{1}$ for every j , $E_j = L$ for $j = k$ and $E_j = 0$ otherwise, and $f_j(x) = x$, for every j . To prove 2., we need to prove that: (a) $iH \in i \text{ Sim } \Leftrightarrow -iH \in i \text{ Sim }$; (b) $iH \in i \text{ Sim } \Rightarrow aiH \in i \text{ Sim }$, for each positive a ; (c) $iH_1, iH_2 \in i \text{ Sim } \Rightarrow i(H_1 + H_2) \in i \text{ Sim }$; (d) $iH_1, iH_2 \in i \text{ Sim } \Rightarrow [iH_1, iH_2] \in i \text{ Sim }$. That is, (a), (b) and (c) show that $i \text{ Sim }$ is a vector space and (d) that is closed under commutation relation. Rewrite (39) as

$$e^{-iHx} = T(x) + O(x^{1+\delta}), \quad (46)$$

(cf. (45)), i.e., by replacing the product in (39) by the symbol $T(x)$, and notice that $T^{-1}(x)$ can be also written as a product of the form in (39). By straightforward manipulations of (46) we obtain $T^{-1}(x) = e^{iHx} + T^{-1}(x)O(x^{1+\delta})e^{iHx}$, that is $e^{iHx} = T^{-1}(x) + O(x^{1+\delta})$, which shows (a). To show (b), notice that if $T(x)$ is an admissible product so is $T(ax)$, for $a > 0$, so by replacing x with ax in (46), we obtain the result. To prove (c), denote by $T_1(x)$ and $T_2(x)$ the product in (46) corresponding to H_1 and H_2 , respectively and δ_1 and δ_2 , the corresponding δ 's in (46). From the exponential formula $e^{-iH_1x}e^{-iH_2x} = e^{-i(H_1+H_2)x} + O(x^2)$, we obtain

$$e^{-i(H_1+H_2)x} + O(x^2) = (T_1(x) + O(x^{1+\delta_1})) (T_2(x) + O(x^{1+\delta_2})),$$

which gives

$$e^{-i(H_1+H_2)x} = T_1(x)T_2(x) + O(x^{1+\min(1,\delta_1,\delta_2)}).$$

¹⁰All the Lie algebras we are considering are subalgebras of the *real* Lie algebra $u(n)$ (for appropriate n).

which shows our claim since $T_1 T_2$ is also an admissible product. Finally, to prove (d) we use the exponential formula $e^{[-iH_1, -iH_2]t^2} + O(t^3) = e^{-iH_1 t} e^{-iH_2 t} e^{iH_1 t} e^{iH_2 t}$. (see, e.g., [5], Section 6.5.). Using this and the notation described above, call $O_{1,2}$ the O function for H_1 and H_2 , respectively. We have

$$e^{[-iH_1, -iH_2]t^2} + O(t^3) = \\ (T_1(t) + O_1)(T_2(t) + O_2) \left(T_1^{-1}(t) - T_1^{-1}(t)O_1 e^{iH_1 t} \right) \left(T_2^{-1}(t) - T_2^{-1}(t)O_2 e^{iH_2 t} \right).$$

Expanding the right hand side and omitting explicit terms that are clearly $O(t^\alpha)$ for $\alpha > 2$ since they contain products of two O functions, we obtain

$$e^{[-iH_1, -iH_2]t^2} + O(t^3) = O(t^\alpha) + T_1 T_2 T_1^{-1} T_2^{-1} - T_1 T_2 T_1^{-1} T_2^{-1} O_2 e^{iH_2 t} - T_1 T_2 T_1^{-1} O_1 e^{iH_1 t} T_2^{-1} + \\ (47) \\ T_1 O_2 T_1^{-1} T_2^{-1} + O_1 T_2 T_1^{-1} T_2^{-1}.$$

Developing in a Taylor series the functions that multiply the O functions on the right hand side of this expression gives cancelations which show that only terms of the type $O(t^{2+\delta_1})$ and $O(t^{2+\delta_2})$ possibly remain. In conclusion, we have

$$e^{[-iH_1, -iH_2]t^2} = T_1(t) T_2(t) T_1^{-1}(t) T_2^{-1}(t) + O(t^\beta), \quad (48)$$

with $\beta > 2$ and by setting $x = t^2$, we obtain

$$e^{[-iH_1, -iH_2]x} = T_1(\sqrt{x}) T_2(\sqrt{x}) T_1^{-1}(\sqrt{x}) T_2^{-1}(\sqrt{x}) + O(x^{\frac{\beta}{2}}), \quad (49)$$

which show the result because if $T(x)$ is an admissible product so is $T(\sqrt{x})$. This concludes the proof of the theorem. \square

5 Example

I consider now an example of a coined DTQW whose associated CTQW can be obtained as an appropriate limit. This example is not a DTQW on cycle or d -lattice and shows the generality of the method described above. In particular, consider the graph in Figure 1 which has a three dimensional coin space \mathcal{C} (spanned by the coin tossing results 1, 2, 3) and a 4-dimensional walker space spanned by the positions A, B, C, D , in that order.

The associated matrix S is given by $S = \text{diag}(S_1, S_2, S_3)$, with

$$S_1 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \quad S_2 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \quad S_3 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}. \quad (50)$$

The Lie algebra of simulable Hamiltonians $i \text{Sim}$ is generated by

$$\mathcal{F} = \{u(3) \otimes \mathbf{1}_4, Su(3) \otimes \mathbf{1}_4 S\}, \quad (51)$$

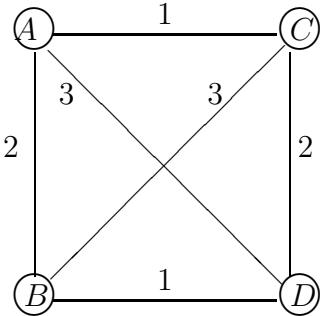


Figure 1: Graph for the discrete time quantum walk in the example. The labels on the edges indicate the corresponding coin toss result. In this example the same coin toss result induces motion in both directions.

since S has order 2. It contains, in particular, the element $\text{diag}(-3i, i, 2i) \otimes \mathbf{1}_4$. The adjacency matrix $A := S_1 + S_2 + S_3$ has one eigenvalue equal to 3 with multiplicity 1 and one eigenvalue -1 with multiplicity 3. Therefore, we can single out a 4-dimensional vector space of $\mathcal{C} \otimes \mathcal{V}$ of the DTQW where the dynamics coincide with the one of the CTQW corresponding to the adjacency matrix. We can, in fact, do better by studying more closely the structure of the Lie algebra generated by \mathcal{F} in (51). S_1 , S_2 and S_3 can be simultaneously diagonalized, and moreover we have $S_1 S_2 = S_3$, $S_2 S_3 = S_1$ and $S_3 S_1 = S_2$ and $S_1^2 = S_2 = S_3^2 = \mathbf{1}_4$. The set \mathcal{F} can be written as

$$\mathcal{F} = \{u(3) \otimes \mathbf{1}_4, E_{12} \otimes S_3, E_{13} \otimes S_2, E_{23} \otimes S_1, \} \quad (52)$$

where E_{jk} represents the set of all the matrices in $su(3)$ with all the entries equal to zero except for the j, k and j, k entries. From this, one finds that

$$\mathcal{L} = \text{span } \{u(3) \otimes \mathbf{1}_4, su(3) \otimes S_1, su(3) \otimes S_2, su(3) \otimes S_3.\} \quad (53)$$

It is in fact clear that this is a Lie algebra containing \mathcal{F} . Moreover by calculating the set $\bigoplus_{k=0}^{\infty} ad_{su(3)}^k E_{jk}$, for a given jk it is clear that this is all of $su(3)$, since it is a non-empty ideal in $su(3)$, which is a simple Lie algebra. Therefore, we obtain with repeated Lie brackets all the matrices in $su(3) \otimes S_{1,2,3}$. At this point, it is convenient to make a change of coordinates to simultaneously diagonalize S_1 , S_2 and S_3 and to change the order of the tensor product in (53). Therefore the matrices in \mathcal{L} are linear combinations of matrices of the form $L_1 := \text{diag}(A, A, A, A)$, $L_2 := \text{diag}(B, B, -B, -B)$, $L_3 := \text{diag}(-C, C, -C, C)$, $L_4 := \text{diag}(-D, D, D, -D)$, with $A \in u(3)$, and $B, C, D \in su(3)$. We can choose a linear

combination of $L_{1,2,3,4}$ to make the resulting matrix have eigenvalues $\pm 3i$ with multiplicity 1 and $\pm i$ with multiplicity 3 and 0 with multiplicity 4, so as to obtain 2 copies of the CTQW (one backward and one forward in time) and no dynamics on appropriate four dimensional subspaces of $\mathcal{C} \otimes \mathcal{V}$.

6 Conclusions

I have obtained the dynamics of the continuous time quantum walk on the cycle as an appropriate limit of the coined discrete time quantum walk on the same graph. This result can be extended directly to the case of d -lattices using the fact that they are products of cycles. The main ideas of the procedure can be extended to general graphs. One can use the discrete time quantum walks to obtain the dynamics corresponding to a given Hamiltonian on the whole (coin+walker) space and then obtain the dynamics of the continuous time quantum walk by restricting oneself to a subspace of the whole (coin+walker) space. I have characterized the set of Hamiltonians for which this is possible, a set that I called of simulable Hamiltonians. The results of this paper reduce the problem of obtaining the continuous time quantum walk from the discrete time to the problem to a study of the set of simulable Hamiltonians. This set has the structure of a Lie algebra. As this set is quite rich it is reasonable to expect that every (or at least most) continuous time quantum walks can be obtained by a limiting procedure and restricting to an appropriate subspace the dynamics of the associated discrete time quantum walk.

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